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Calculation of low-field chemical shifts for α-CH protons in native and compact denatured binase

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Abstract

Crystallographic data on binase and models of internal electric and magnetic fields were used to calculate the chemical shift dispersion (CSD) for α-CH protons of residues in β-regions. Fitting parameters were found describing the internal fields of peptide groups and permitting conciliation of the theoretical and experimental CSD for native protein. The same models were used to assess the behavior of proton CSD upon binase transition to a compact denatured state. It was shown that disappearance of low-field 1H NMR lines of α-CH protons does not indicate disruption of secondary-structure elements, but can be explained by fluctuations in the H-bond network caused by pronounced intramolecular dynamics.

Keywords

1H NMR spectroscopy, Binase, Compact denatured state, Protein structure, Proton chemical shift